ABSTRACT

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Title of Diploma Thesis: Optimization of SFC method for chiral screening

Method for effective chiral screening was developed for 37 chiral pairs of compounds of different structures and acid-base properties. Measurement was performed on SFC system Acquity UPC^2 with PDA detector, using chiral polysacharides columns with particles 2.5 µm or 3 µm. Mobile phase flow was set to 2.0 ml/min due to the maximum pressure limits of most of the tested columns. Gradient elution with column temperature set to 40°C and ABPR pressure of 12 MPa was used. For primary screening 10 mobile phases were chosen, from which 2 best were used for all of the tested columns.

An equivalence of columns with the same chiral selectors phase from different manufacturers was not confirmed. Considering the complexity of chiral recognition mechanisms general rules for the choice of the columns or mobile phase could not been clearly defined. Chiralcel OD-3 with IPA + 0.1% TFA,DEA was column with the most separated enantiomers. Chiralcel OD-3 with MeOH + 0.1% TFA,DEA was the best column considering overall percentual scale including the resolution and peak shape. Thus was formed to be the Chiralcel OD-3 the most generic column with use of tested modifiers.

Keywords: Supercritical fluid chromatography, column evaluation, chiral separations, screening, amylose, cellulose, stationary phase, chiral selector